Optimal Proton Trapping Strategy for a Neutron Lifetime Experiment

Kevin J. Coakley a,*

^aStatistical Engineering Division, National Institute of Standards and Technology, 325 Broadway, Boulder C0 80305 fax: 303 497 3012 phone: 303 497 3895

Abstract

In a neutron lifetime experiment conducted at the National Institute of Standards and Technology, protons produced by neutron decay events are confined in a proton trap. In each run of the experiment, there is a trapping stage of duration τ . After the trapping stage, protons are purged from the trap. A proton detector provides incomplete information because it goes dead after detecting the first of any purged protons. Further, there is a dead time δ between the end of the trapping stage in one run and the beginning of the next trapping stage in the next run. Based on the fraction of runs where a proton is detected, I estimate the trapping rate λ by the method of maximum likelihood. I show that the expected value of the maximum likelihood estimate is infinite. To obtain a maximum likelihood estimate with a finite expected value and a well-defined and finite variance, I restrict attention to a subsample of all realizations of the data. This subsample excludes an exceedingly rare realization that yields an infinite-valued estimate of λ . I present asymptotically

valid formulas for the bias, root-mean-square prediction error, and standard deviation of the maximum likelihood estimate of λ for this subsample. Based on nominal values of λ and the dead time δ , I determine the optimal duration of the trapping stage τ by minimizing the root-mean-square prediction error of the estimate.

Key words: , Lifetimes,21.10.Tg, Nuclear tests of fundamental interactions and symmetries,24.80+y, Properties of protons and neutrons, 14.20.Dh, Probability theory, stochastic processes, and statistics,02.50-r

1 Introduction

Ion traps play a key role in fundamental physics experiments (Ref. 1). In this paper, I focus on statistical methods for uncertainty analysis and planning of proton trap neutron lifetime experiments (Refs. 1-5) and related experiments such as Ref. 6. When a neutron decays, it produces a proton, an electron and an antineutrino. An accurate determination of the mean lifetime of the neutron is critically important for testing the fundamental theories of physics (Ref. 7). Further, the mean lifetime of the neutron is an important parameter in the astrophysical theory of big bang nucleosynthesis (Ref. 8). In a proton trap neutron lifetime experiment performed at the National Institute of Standards and Technology (NIST), a beam of neutrons passes through a detection volume. Based on measurements of the neutron flux and the proton production rate, one measures the mean lifetime of the neutron. Each run of the experiment consists of trapping stage where protons are confined in a trap (Refs. 2-5),

Email address: kevin.coakley@nist.gov (Kevin J. Coakley).

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and a detection stage. The detector provides incomplete information because it goes dead after detecting the first proton. Based on the number of runs where a proton is detected, one can estimate the proton trapping rate.

In earlier work [Ref. 9], this estimation problem was studied using a Bayesian method. Given a particular realization of the data (the number of runs where at least one ion (proton in this paper) is trapped), a formula for the posterior mean of the ion trapping rate was presented based on a prior probability model for the trapping rate. In this work, I estimate the trapping rate by the method of maximum likelihood and focus on the statistical properties of this estimate. I neglect physical sources of systematic error due to effects such as a time varying proton trapping rate or fluctuations in the actual trapping stage interval about the nominal value sought by the experimenter.

In Section 2, I demonstrate that the bias (expected value minus true value) and variance of the maximum likelihood estimate of the trapping rate λ are infinite. This is so because a rare realization of the data yields an infinite estimate of λ . This technical problem can be dealt with in various ways. One could quantify uncertainty by constructing confidence intervals of finite width even though the variance of the estimate is infinite. Another approach would be to introduce a stopping rule so that the experiment is continued until no protons are trapped in at least one run. I do not pursue either of these approaches here. Instead, I restrict the sample space to include only realizations of data where one observes at least one run where no protons are trapped. For realizations of data in this subsample, the maximum likelihood estimate has finite first and second moments. In Section 3, I derive asymptotically valid formulas for the bias, variance, and mean-square-error of a maximum likelihood estimate of the proton trapping rate computed from this subsample. In general, one

expects estimates that are nonlinear functions of the observed data, such as the maximum likelihood estimate of the trapping rate, to be biased [Ref. 10]. In Section 4, where, based on nominal values of trapping rate and dead time, I determine the trapping time that minimizes the root-mean-square prediction error of the maximum likelihood estimate of λ in the subsample of interest.

2 Statistical Model

In a simulated proton trapping experiment there are many runs. During each run, I assume that the duration of the proton trapping stage τ is an adjustable constant that is known with negligible uncertainty. During the trapping stage, I assume that protons are trapped at a constant rate λ . Further, I restrict attention to the case where $\lambda > 0$. After the trapping stage, protons are purged from the trap. A proton detector provides incomplete information because it goes dead after detecting the first of any purged protons. Further, there is a fixed dead time δ between the end of the trapping stage in one run and the beginning of the next trapping stage in the next run. I assume that δ is known with negligible uncertainty. If the total time of the experiment is T, the total number of runs is

$$N_{run} = INT(\frac{T}{\tau + \delta}). \tag{1}$$

Above, the function INT(x) rounds the continuous variable x down to the nearest integer. Let n_+ be the observed number of runs where at least one proton is trapped. I model the number of protons trapped during any run as a realization of a Poisson process with expected value $\lambda \tau$. Hence, the probability that no ion is trapped for a given run is

$$p_0 = \exp(-\lambda \tau). \tag{2}$$

The maximum likelihood estimate of p_0 is

$$\hat{p}_o = 1 - \frac{n_+}{N_{run}} \tag{3}$$

where n_{+} is the number of runs where at least one proton is trapped. Thus, the maximum likelihood estimate of λ is

$$\hat{\lambda} = -\frac{1}{\tau} \ln \hat{p}_0 = -\frac{1}{\tau} \ln(1 - \frac{n_+}{N_{run}}). \tag{4}$$

Since n_+ is a binomial random variable, the probability that $n_+ = k$ is P(k), where

$$P(k) = \frac{N_{run}!}{(N_{run} - k)!k!} (1 - p_0)^k p_0^{N_{run} - k}.$$
 (5)

Hence, the expected value of the maximum likelihood estimate of λ is

$$E(\hat{\lambda}) = -\frac{1}{\tau} \sum_{k=0}^{N_{run}} P(k) \ln(1 - \frac{k}{N_{run}}).$$
 (6)

Similarly, the expected squared value of the estimate is

$$E(\hat{\lambda}^2) = \frac{1}{\tau^2} \sum_{k=0}^{N_{run}} P(k) \left(\ln\left(1 - \frac{k}{N_{run}}\right)\right)^2.$$
 (7)

For $\lambda > 0$, $P(N_{run}) = (1 - p_0)^{N_{run}} > 0$, and both the expected value (first moment) and expected squared value (second moment) of $\hat{\lambda}$ are infinite. The variance of $\hat{\lambda}$, $VAR(\hat{\lambda})$, is not defined because

$$VAR(\hat{\lambda}) = E(\hat{\lambda}^2) - (E(\hat{\lambda}))^2, \tag{8}$$

and both terms on the right hand side of Eq. 8 are infinite.

To ensure that both $E(\hat{\lambda})$ and $E(\hat{\lambda}^2)$ are finite, I restrict the sample space to realizations of the data where $n_+ < N_{run}$. From a practical point of view, this means that realizations of data where $n_+ = N_{run}$ would be ignored. For neutron lifetime experiments of current interest, the probability that $n_+ = N_{run}$ is negligible provided that τ is judiciously chosen. Hence, this subsampling restriction does not significantly affect data collection procedures for neutron lifetime experiments of current interest. In this subsample, the discrete probability density function for allowed realizations of $n_+ = 0, 1, \dots, N_{run} - 1$ is $P_*(k)$, where

$$P_*(k) = \frac{P(k)}{1 - P(N_{run})}. (9)$$

For this subsample, the first two moments of the maximum likelihood estimate are

$$E(\hat{\lambda}) = -\frac{1}{\tau} \sum_{k=0}^{N_{run}-1} P_*(k) \ln(1 - \frac{k}{N_{run}}), \tag{10}$$

and

$$E(\hat{\lambda}^2) = \frac{1}{\tau^2} \sum_{k=0}^{N_{run}-1} P_*(k) (\ln(1 - \frac{k}{N_{run}}))^2.$$
 (11)

Since the first two moments (Eqns. 10 and 11) of $\hat{\lambda}$ are finite, the variance of $\hat{\lambda}$ is defined and finite. Next, I present analytical formulas to approximate the fractional bias, fractional standard deviation and fractional root-mean-square prediction error of the estimate computed for this subsample.

3 Asymptotic Approximations for Analysis in Subsample

In the subsample where $n_+ < N_{run}$, I derive asymptotically valid approximations for the fractional bias (FBIAS), fractional root-mean-square prediction error (FRMS), and fraction standard deviation (FSE) of $\hat{\lambda}$ where

$$FBIAS = \frac{E(\hat{\lambda} - \lambda)}{\lambda},\tag{12}$$

$$FRMS = \frac{\sqrt{E(\hat{\lambda} - \lambda)^2}}{\lambda},\tag{13}$$

and

$$FSE = \frac{\sqrt{E(\hat{\lambda} - E(\hat{\lambda}))^2}}{\lambda} = \sqrt{(FRMS)^2 - (FBIAS)^2}.$$
 (14)

To facilitate analysis of $\hat{\lambda}$ in the subsample I write

$$\hat{p}_0 = p_0 - \epsilon = p_0 \left(1 - \frac{\epsilon}{p_0}\right),\tag{15}$$

$$\epsilon = p_0 - \hat{p}_0. \tag{16}$$

Thus,

$$\ln \hat{p}_0 = \ln(p_0) + \ln(1 - w) \tag{17}$$

where

$$w = \frac{\epsilon}{p_0}. (18)$$

In the subsample, w takes discrete values in the following interval

$$1 - \frac{1}{p_0} \le w \le 1 - \frac{1}{N_{run}p_0}. (19)$$

The BIAS of the maximum likelihood estimate of λ in the subsample is

$$BIAS = -\tau^{-1}(E(\ln \hat{p}_0) - \ln(p_0)) = -\tau^{-1}E(\ln(1-w))$$
(20)

where w is a random variable.

I derive an asymptotically valid expression for BIAS based on a local approximation for $\ln(1-w)$ in the vicinity of 0. I approximate $f(w) = -\ln(1-w)$ as a fourth order polynomial $\hat{f}(w)$ where

$$\hat{f}(w) \approx f(0) + wf^{1}(0) + \frac{w^{2}}{2!}f^{2}(0) + \frac{w^{3}}{3!}f^{3}(0) + \frac{w^{4}}{4!}f^{4}(0)$$
(21)

where $f^k(0)$ is the kth derivative of f(w) evaluated at w=0. Thus,

$$\hat{f}(w) = \sum_{k=1}^{4} \frac{w^k}{k} = \sum_{k=1}^{4} \frac{\epsilon^k}{k(p_0)^k}.$$
 (22)

Since

$$\epsilon = \frac{n_+ - E(n_+)}{N_{run}},\tag{23}$$

the central moments $\mu_r = E((n_+ - E(n_+))^r)$ are relevant. In the full sample where $n_+ \leq N_{run}$, n_+ is a binomial random variable with an expected value equal to $N_{run}(1-p_0)$. Hence, in full sample, its first four central moments are [11]

$$\mu_1 = 0, \tag{24}$$

$$\mu_2 = N_{run} p_0 (1 - p_0), \tag{25}$$

$$\mu_3 = N_{run}p_0(1 - p_0)(2p_0 - 1), \tag{26}$$

and

$$\mu_4 = 3N_{run}^2 p_0^2 (1 - p_0)^2 + N_{run} p_0 (1 - p_0) (1 - 6p_0 (1 - p_0)). \tag{27}$$

Since $P(n_+ = N_{run})$ tends to 0 exponentially as a function of N_{run} , the asymptotic central moments of n_+ in the subsample are given by Eqns. 24-27.

Based on Eqns. 22,25,26 and 27, I get the following approximation for FBIAS

$$\widehat{FBIAS} \approx \frac{1}{\lambda \tau} \left[\frac{\mu_2}{2(N_{run}p_0)^2} + \frac{\mu_3}{3(N_{run}p_0)^3} + \frac{\mu_4}{4(N_{run}p_0)^4} \right].$$
 (28)

In a similar calculation where I approximate f(w) as a second order polynomial, I get the following approximation for FRMS

$$\widehat{FRMS} \approx \frac{1}{\lambda \tau} \sqrt{\frac{\mu_2}{(N_{run}p_0)^2} + \frac{\mu_3}{(N_{run}p_0)^3} + \frac{\mu_4}{4(N_{run}p_0)^4}}.$$
 (29)

From Eqns. 28 and 29, I derive an approximation for FSE

$$\widehat{FSE} = \sqrt{(\widehat{FRMS})^2 - (\widehat{FBIAS})^2}.$$
(30)

Since the asymptotic standard deviation of the random variable w is

$$\sigma_w = \sqrt{\frac{1 - p_0}{N_{run}p_0}},\tag{31}$$

I expect Eqns. 28-30 to be asymptotically valid as N_{run} increases to large values. Next, I present evidence consistent with this expectation for a number of cases (Tables 1,2).

4 Example

For particular cases, I compute the actual values of FRMS, FBIAS and FSE using Eqns. 9-14. I set $\delta=100~\mu\mathrm{s}$ (0.0001 s) and $\lambda=1$ Hz because these are typical values for experiments done at NIST. For experiments of total duration of $T=10~\mathrm{s}$, 25 s, 50 s, 100 s, 200 s, and 400 s, FBIAS was much less than FRMS (see Figure 1 and Table 1). Furthermore, FBIAS was more sensitive to τ than FRMS was (Figure 1). For the cases summarized in Table 1, the fractional systematic error and fractional RMS prediction error are well approximated as $FBIAS \propto T^{-1}$, and $FRMS \propto T^{-1/2}$. For each cases, both FRMS and \widehat{FRMS} (Eqn. 29) took their minimum values at $\tau=0.014~\mathrm{s}$. The resolution of the grid on which I computed RMS prediction errors is 0.001 s in the neighborhood of the 0.014 s.

In a second simulation, I set T=400 s and $\lambda=100$ Hz. I vary τ so that the expected number of trapped protons per run, $\lambda \tau$, varies from .001 to 4. For these cases, \widehat{FBIAS} and \widehat{FRMS} closely track the actual values of FBIAS and FRMS (Table 2). For the smallest values of τ , the accuracies of the approximations are highest. I attribute the slight degradation of approximation accuracy at the largest values of $\lambda \tau$ to the fact that σ_w (Eq. 31) is a monotonically increasing function of τ .

For convenience, I express the fractional RMS prediction error of $\hat{\lambda}$ as

$$FRMS = 0.001\sqrt{\frac{T^*}{T}},\tag{32}$$

where T is the total time of the experiment. The parameter T^* is a function of λ , τ and δ . In proton trap neutron lifetime experiments, λ depends on exper-

imental details including the length of the trap; trapping efficiency; and the neutron flux (Refs. 2-5) For the cases considered here, I compute T^* directly using Eqns. 9-14 and Eq. 32. For fixed values of λ , δ , and τ , the derived value of T^* is approximately the same for all values of T. An exception to this rule is when δ is large and there are very few bins. I attribute this to truncation effects associated with rounding N_{run} to an integer (Eq. 1). Thus, one can compute T^* from simulation data corresponding to one sufficiently large value of T and predict FRMS at other large values of T. As a caveat, for very short experiments, the asymptotic theory may not apply and a direct simulation may be necessary.

For the case where the dead time δ is fixed, T^* varies as a function of both λ and τ (Figure 2) in a complicated manner. To clarify resutls, I scale T^* and τ by the true trapping rate λ (Figure 3). I define τ_{opt} to be the value of τ that minimizes FRMS. Based on Figure 3, the most elucidating way to find the optimal data collection strategy is to minimize λT^* as a function of $\lambda \tau$. For the cases shown in Figures 2 and 3, I conclude that $\lambda \tau_{opt}$ increases as λ increases. In a second simulation experiment, I consider cases where λ is fixed but the dead time δ varies from case to case. For these cases, as δ increases, so too does $\lambda \tau_{opt}$ (Figure 4).

5 Discussion

Earlier I stated that the subsample restriction has no practical effect on data collection for neutron lifetime experiments of current interest. To make this claim more concrete, I compute the probability of observing $n_+ = N_{run}$ in the full sample for the cases listed in Table 1. For these cases, $\tau = 0.014$ s and $\lambda = 0.014$ s and $\lambda = 0.014$ s and $\lambda = 0.014$ s.

1 s⁻¹ and $P(N_{run}) \approx 10^{-1.8569N_{run}}$. Hence for an experiment of total duration 100 s, $P(N_{run}) \approx 10^{-13169}$.

In the study, I quantified FBIAS given knowledge of λ and particular values of τ , δ and T. In actual experiments, one would use the estimated value of λ rather than the true value. Hence, in Eqn. 28, one would use $\hat{p}_0 = \exp(-\hat{\lambda}\tau)$ rather than the true value of p_0 . If FBIAS is negligible, there is no need to correct $\hat{\lambda}$ for bias. In principle, when bias is significant, a bias-corrected maximum likelihood estimate should be obtained using the following iterative procedure:

$$\hat{\lambda}_{(k+1,BC)} = \frac{\hat{\lambda}}{1 + \widehat{FBIAS}(\hat{\lambda}_{(k,BC)}, N_{run}, \tau)}$$
(33)

where $\hat{\lambda}_{(0,BC)} = \hat{\lambda}$ and $\hat{\lambda}_{(k+1,BC)}$ is the bias-corrected maximum likelihood estimate at the kth iteration. In practice, one iteration of the above procedure may yield a numerically stable estimate of the bias-corrected maximum likelihood estimate for cases of interest.

6 Summary

In this work, I studied the statistical properties of a maximum likelihood estimate of the rate at which protons are trapped. This study is relevant to proton trap neutron lifetime experiments at NIST and similar experiments elsewhere. After the first proton is detected, the detector goes dead. Hence, the detector provides incomplete information. Due to this incompleteness, I showed that the first two moments of the maximum likelihood estimate of the trapping rate λ are infinite. Hence, the variance of the maximum likelihood

estimate is not defined. To construct a maximum likelihood estimate with a finite variance, I restricted attention to a subsample of realizations of the data that excludes an exceedingly rare realization of the data that yields an infinite valued estimate of λ . I demonstrated that the probability of observing this rare realization quickly decreases to a negligible value for a judicious choice of the trapping time for proton trapping rates achievable at NIST (Secion 5). Hence, restricting attention to the subsample of interest has no practical effect on current neutron lifetime experiments of interest. Based on the discrete probability density function for this subsample, I derived exact formulas for the first two moments of the maximum likelihood estimate of λ (Eqns. 10 and 11). I derived asymptotically valid formulas for the fractional bias, fractional RMS prediction error and fractional standard deviation of the maximum likelihood estimate (Eqns. 28-30). I showed that the approximation error associated with these formulas is low for a variety of cases (Tables 1,2).

I demonstrated that the fractional bias (FBIAS) of the estimate was more sensitive to τ than the fractional mean-square prediction error (FRMS) was (Figure 1). As as a function of total observing time T, I showed that FBIAS decreases much faster than does FRMS (Table 1).

I presented an objective method to select the optimal value of τ by minimizing FRMS. In general, the optimal trapping time τ that minimizes FRMS is a complicated function of both dead time δ and the trapping rate λ (Figures 2-4). For experimental planning purposes, my asymptotic approximations (Eqns. 28-30) should be useful for determining the optimal data collection strategy and for quantifying random and systematic errors.

In this study, I neglected physical sources of systematic error due to effects such

as a time varying proton trapping rate or fluctuations in the actual trapping stage interval about the nominal value sought by the experimenter. Hence, the bias I quantified here is a purely statistical artifact due to the fact the maximum likelihood estimate of the trapping rate is a nonlinear function of the observed data.

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Table 1. Proton trapping rate is $\lambda=1~{\rm s}^{-1}$. Dead time is $\delta=0.0001~{\rm s}$. Trapping stage duration is $\tau=0.014~{\rm s}$. FRMS and FBIAS are fractional bias and fractional root-mean-square prediction error of the maximum likelihood estimate of λ . The approximations for \widehat{FRMS} and \widehat{FBIAS} are computed using Eqns. 28 and 29.

| T (s) | N_{run} | $E(n_+)$ | FBIAS | \widehat{FBIAS} | FRMS | \widehat{FRMS} |
|-------|-----------|----------|-------------|-------------------|-----------|------------------|
| 10 | 709 | 9.85684 | 0.000710859 | 0.000710858 | 0.318749 | 0.318742 |
| 25 | 1773 | 24.6491 | 0.0002841 | 0.0002841 | 0.201479 | 0.201477 |
| 50 | 3546 | 49.2981 | 0.000142023 | 0.000142023 | 0.142446 | 0.142446 |
| 100 | 7092 | 98.5962 | 7.10046e-05 | 7.10046e-05 | 0.100717 | 0.100717 |
| 200 | 14184 | 197.192 | 3.55006e-05 | 3.55006e-05 | 0.0712154 | 0.0712154 |
| 400 | 28368 | 394.385 | 1.77499e-05 | 1.77499e-05 | 0.050356 | 0.050356 |

Table 2. Simulation study. Proton trapping rate is $\lambda=100~{\rm s}^{-1}.$ Dead time is $\delta=0.0001~{\rm s}.$ $T=400~{\rm s}.$

| τ (s) | $\lambda 	au$ | N_{run} | $E(n_+)$ | FBIAS | \widehat{FBIAS} | FRMS | \widehat{FRMS} |
|------------|---------------|-----------|----------|-------------|-------------------|------------|------------------|
| 1e-05 | 0.001 | 3636360 | 3634.55 | 1.37569e-07 | 1.37569e-07 | 0.0165873 | 0.0165873 |
| 1e-04 | 0.01 | 2e + 06 | 19900.3 | 2.51254e-07 | 2.51254e-07 | 0.00708878 | 0.00708878 |
| 0.001 | 0.1 | 363636 | 34604.5 | 1.4461e-06 | 1.4461e-06 | 0.00537793 | 0.00537793 |
| 0.01 | 1 | 39603 | 25033.9 | 2.1695 e-05 | 2.1695e-05 | 0.00658726 | 0.00658698 |
| 0.015 | 1.5 | 26490 | 20579.3 | 4.38173e-05 | 4.38173e-05 | 0.007644 | 0.007643 |
| 0.02 | 2.0 | 19900 | 17206.8 | 8.02887e-05 | 8.02887e-05 | 0.00896179 | 0.00895891 |
| 0.03 | 3.0 | 13289 | 12627.4 | 0.000239664 | 0.000239664 | 0.0126488 | 0.0126306 |
| 0.04 | 4.0 | 9975 | 9792.3 | 0.000674739 | 0.000674717 | 0.0184136 | 0.0183143 |

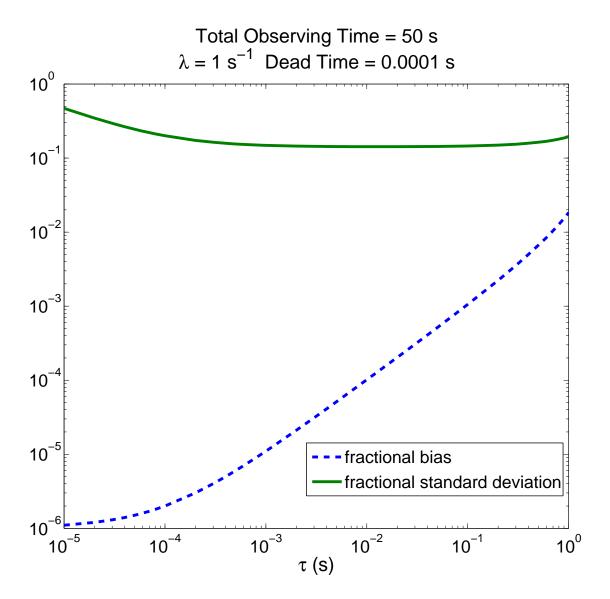


Figure 1. Fractional bias (FBIAS) and fractional standard error (FSE) for simulation experiment where true trapping rate is $\lambda = 1 \text{ s}^{-1}$, total duration of experiment is T = 50 s, dead time is $\delta = 100 \ \mu\text{s}$, and trapping stage duration τ varies.

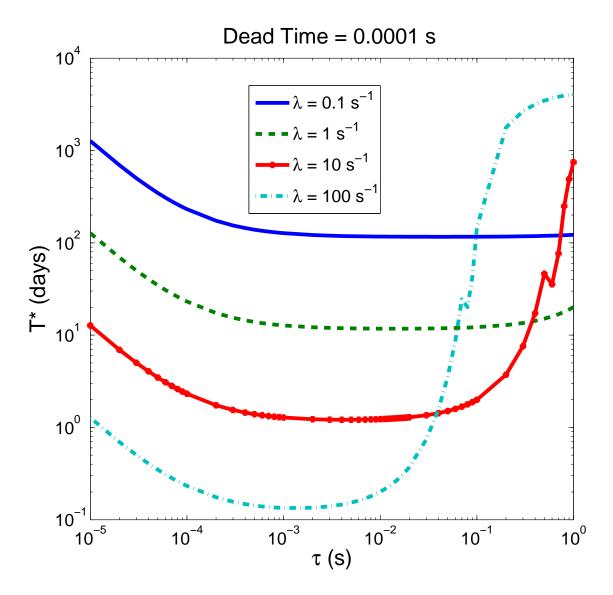


Figure 2. Fractional RMS prediction error (FRMS) of the trapping rate is expressed as $0.001\sqrt{\frac{T^*}{T}}$, where the total length of the experiment is T. Dead time is $\delta = 0.0001$ s.

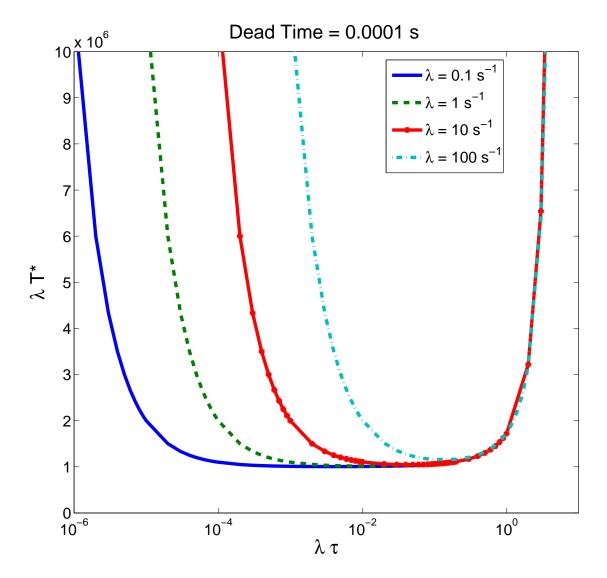


Figure 3. Same results as in Figure 2, but T^* and τ are rescaled to clarify results.

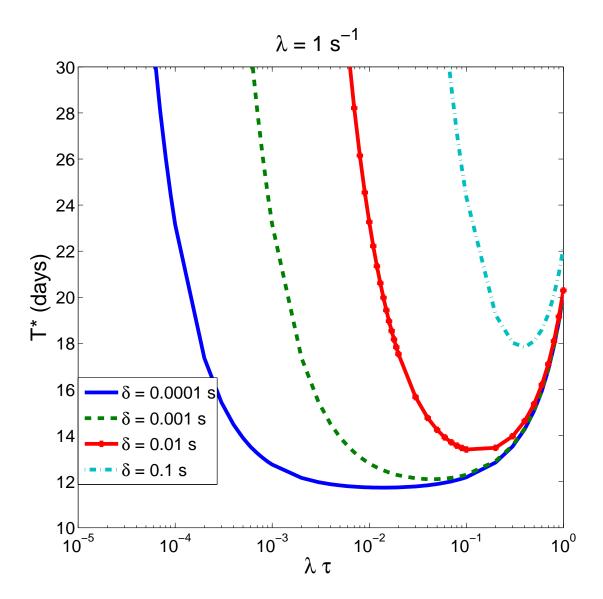


Figure 4. True proton trapping rate is $\lambda = 1 \text{ s}^{-1}$.